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UNITED STATES
ENVIRONMENTAL PROTECTION AGENCY
HIGH PRODUCTION VOLUME
CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

1-Decene, Tetramer, Mixed with 1-Decene Trimer, Hydrogenated
CAS # 68649-12-7

Prepared by:

American Chemistry Council
Higher Olefins Panel, Polyalphaolefins Task Group

October 4, 2002

EXECUTIVE SUMMARY

The Higher Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the test plan for 1-decene, tetramer, mixed with 1-decene trimer, hydrogenated (decene tetramer/trimer), CAS number 68649-12-7, under the United States Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program). The Panel's member companies have committed to identify or develop sufficient screening level test data and other information to adequately characterize the HPV Program human health effects, physicochemical, and environmental fate and effects endpoints for decene tetramer/trimer.

Decene tetramer/trimer is a long chain branched alkane (a hydrogenated polyalphaolefin [PAO]). The predominant (~85%) and shortest oligomer present is a C30 (carbon number 30), with a C40 oligomer comprising most of the remainder.

Read across data exist for all HPV Program health effects endpoints from similar long chain branched alkanes. The data for these structural analogs, derived from C8, C10 and/or C12 alpha olefins, demonstrated no evidence of health effects. In addition, there is evidence in the literature that alkanes with 30 or more carbon atoms are unlikely to be absorbed when administered orally. These data are considered to be sufficient to adequately characterize the HPV Program human health effects endpoints and no further health effects testing is proposed.

Data exist from aquatic toxicity and aerobic biodegradation studies with decene tetramer/trimer and for a C8/C10/C12 PAO (1-octene, 1-decene, 1-dodecene copolymer, hydrogenated). The aquatic studies showed that these PAOs did not produce acute toxicity. The lack of aquatic toxicity is likely due to water solubility limitations. The biodegradation data suggest that decene tetramer/trimer, although it does not meet the criteria to be considered readily biodegradable, can biodegrade to a great extent. Therefore, decene tetramer/trimer should not persist in the environment. These data are considered to be sufficient to adequately characterize the HPV Program aquatic toxicity and biodegradation endpoints for this product, and no further testing is proposed for these endpoints.

Data and/or information to adequately characterize photodegradation, photolysis, hydrolysis, and fugacity endpoints and to develop a physicochemical dataset will be identified and/or developed and summarized in robust summaries.

American Chemistry Council's

HIGHER OLEFINS PANEL, POLYALPHAOLEFINS TASK GROUP

The Higher Olefins Panel, Polyalphaolefins Task Group includes the following member companies:

LIST OF MEMBER COMPANIES

Chevron Phillips Chemical Company LP

ExxonMobil Chemical Company

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TEST PLAN FOR 1-DECENE, TETRAMER, MIXED WITH 1-DECENE TRIMER, HYDROGENATED

I. INTRODUCTION

The Higher Olefins Panel (Panel), Polyalphaolefin Task Group (PAO Task Group) of the American Chemistry Council and the Panel's member companies have committed to identify or develop sufficient screening level test data and other information to adequately characterize the HPV Program human health effects, physicochemical, and environmental fate and effects endpoints for 1-decene, tetramer, mixed with 1-decene trimer, hydrogenated (decene tetramer/trimer, CAS number 68649-12-7), under the United States Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program (Program).

This plan identifies:

- Existing data of adequate quality for decene tetramer/trimer,
- Read across data from structural analogs of this chemical that can be used to characterize selected HPV Program endpoints, and
- Information needed to complete the HPV Program data set for this chemical.

II. BACKGROUND

Decene tetramer/trimer and related polyalphaolefins (PAO) are highly branched isoparaffinic chemicals produced by oligomerization of 1-octene, 1-decene, and/or 1-dodecene. To accomplish this, the alpha olefin fractions are mixed with catalysts in continuous reactors under mild temperature and pressure. Treatment of the reactor effluent removes the catalyst residues. The crude polyalphaolefin mixture is then distilled into appropriate product fractions to meet specific viscosity specifications and hydrogenated. Decene tetramer/trimer is a mixture of hydrogenated oligomers prepared from 1-decene with a viscosity of 4 cSt. The typical composition of decene tetramer/trimer is approximately 85% decene trimer, 13% decene tetramer, and 2% decene pentamer and higher.

A significant amount of toxicity data exists for other structurally analogous fractions (products) distilled from crude polyalphaolefin. These data may be used to characterize the HPV Program endpoints for decene tetramer/trimer. The identification and typical compositions of these structural analogs of decene tetramer/trimer are presented below:

Substance	Composition
1-Decene homopolymer, hydrogenated [decene homopolymer] (CAS 68037-01-4)*	Hydrogenated homopolymer prepared from 1-decene [approximately 5% C10 trimer (C30), 49% C10 tetramer (C40) and 46% C10 pentamer (C50) and higher
1-Decene/1-dodecene copolymer, hydrogenated [decene/dodecene copolymer] (CAS 151006-60-9)*	Hydrogenated copolymer prepared from 10% 1-dodecene and 90% 1-decene [C10 oligomers: approximately 33% trimer (C30), 51% tetramer (C40), 16% pentamer (C50) and higher; and C 12 oligomers]

1-Octene, 1-decene, 1-dodecene copolymer, hydrogenated [octene/decene/dodecene copolymer] (CAS 163149-28-8)*	Hydrogenated copolymer prepared from 1-octene, 1-decene, and 1-dodecene
1-Dodecene trimer, hydrogenated [dodecene trimer] (CAS 151006-62-1)*	Hydrogenated trimer prepared from 1-dodecene (C36)

* Not an HPV material

III. EVALUATION OF EXISTING HEALTH EFFECTS DATA

Decene tetramer/trimer is a long chain branched alkane (a hydrogenated polyalphaolefin). The predominant (~85%) and shortest oligomer present is a C30 (carbon number 30), with a C40 oligomer comprising most of the remainder. Read across data exist for all HPV Program health effects endpoints from the following similar long chain branched alkanes derived from a C8, C10, and/or C12 alpha olefins:

- Decene homopolymer
- Decene/dodecene copolymer
- Octene/decene/dodecene copolymer
- Dodecene trimer

The data for these structural analogs of decene tetramer/trimer demonstrated no evidence of health effects. In addition, there is evidence in the literature that alkanes with 30 or more carbon atoms are unlikely to be absorbed when administered orally.

The existing data for analogous substances are considered to be sufficient to adequately characterize the HPV Program human health effects endpoints. No further health effects testing is proposed.

Specific endpoints are addressed below:

A. Mammalian Toxicology Data

1. Physicochemical Properties Relevant to Mammalian Toxicity

The physicochemical data suggest that it is unlikely that significant absorption will occur. If a substance of the size and structure of decene tetramer/trimer is absorbed, then the principal mechanisms of absorption after oral administration are likely to be passive diffusion and absorption by way of the lymphatic system. The former requires both good lipid solubility and good water solubility as the substance has to partition from an aqueous environment through a lipophilic membrane into another aqueous environment during absorption. Absorption by way of the lymphatics occurs by mechanisms analogous to those that absorb fatty acids and is limited by the size of the molecule. Lipophilicity generally enhances the ability of chemicals to cross biological membranes. Biotransformation by mixed function oxidases often increases the water solubility of a substance; however, existing data suggest

that these substances will not undergo oxidation to more hydrophilic metabolites. Finally, a chemical must have an active functional group that can interact chemically or physically with the target cell or receptor upon reaching it. For decene tetramer/trimer, there are no moieties that represent a functional group that may have biological activity.

The water solubilities of a C10 dimer PAO and a C12 trimer PAO were determined to be <1 ppb (Rausina *et al*., 1996) and < 1 ppt (Seary, 2000), respectively. The partition coefficient for a C12 trimer PAO was determined to be Log_{10} P_{ow} of >7 (Seary, 2000). The US EPA EPIWIN model predicts a water solubility of 2.3 x 10^{-10} mg/L and a $Log_{10}P_{ow}$ of 14.62 for decene tetramer/trimer. The calculated octanol/water partition coefficient value for a representative chemical structure used to model white mineral oil (CAS No: 8042-47-5), as supplied in the IUCLID dossier, is reported as >6.

Given the very low water solubility expected for decene tetramer/trimer, it is extremely unlikely that this product will be absorbed by passive diffusion following oral administration, and the size of the molecule suggests that the extent of lymphatic absorption is likely to be very low. Thus, it is unlikely that significant quantities of decene tetramer/trimer would be absorbed when administered orally.

Although decene tetramer/trimer oligomers are relatively large lipophilic compounds, and molecular size may be a critical limiting determinant for absorption, there is some evidence that these substances are absorbed. However, the lack of observed toxicity in the studies with PAOs suggests that these products are absorbed poorly, if at all. Furthermore, a review of the literature regarding the absorption and metabolism of long chain alkanes indicates that alkanes with 30+ carbon atoms are unlikely to be absorbed (Iling [2000], see robust summary). For example, Albro and Fishbein (1970) examined the absorption of squalane, an analogous C30 product, administered orally to male CD rats and found that essentially all of the squalane was recovered unchanged in the feces.

At the same time, the hydrophobic properties of decene tetramer/trimer suggest that, should they be absorbed, they would undergo limited distribution in the aqueous systemic circulation and reach potential target organs in limited concentrations.

In addition to the general considerations discussed above, the low volatility of decene tetramer/trimer indicates that, under normal conditions of use or transportation, exposure by the inhalation route is unlikely. In particular, the high viscosity of these substances suggests that it would be difficult to generate a high concentration of respirable particles in the air.

2. Acute Mammalian Toxicity of Decene Tetramer/Trimer

Summary of Available Data

Acute toxicity data relevant to decene tetramer/trimer are summarized in Table 1. Three structural analogs have been tested for acute oral, dermal and inhalation toxicity. No deaths were observed at or above the limit doses in these tests of long chain branched alkanes similar to decene tetramer/trimer.

Acute Oral Toxicity

Analogous PAOs (decene/dodecene copolymer, octene/decene/dodecene homo-polymer, and dodecene trimer) have been adequately tested for acute oral toxicity. There were no deaths when the test materials were administered at doses of 5,000 mg/kg (decene/dodecene copolymer and dodecene trimer) and at 2,000 mg/kg (octene/decene/dodecene copolymer) in rats. Overall, the acute oral LD_{50} for these substances was greater than the 2000 mg/kg limit dose, indicating a relatively low order of toxicity.

Acute Dermal Toxicity

Analogous PAOs (decene/dodecene copolymer, octene/decene/dodecene copolymer, and dodecene trimer) have been tested for acute dermal toxicity. No mortality was observed for any substance when administered at the limit dose of 2000 or 5000 mg/kg. Overall, the acute dermal LD_{50} for these substances was greater than the 2000 mg/kg limit dose, indicating a relatively low order of toxicity.

Acute Inhalation Toxicity

Analogous PAOs (decene homopolymer, decene/dodecene copolymer, and decene trimer) have been tested for acute inhalation toxicity. Rats were exposed to aerosols of the substances at nominal atmospheric concentrations of 2.5, 5.0, and 5.06 mg/L, respectively, for four hours. These levels were the maximum attainable concentrations under the conditions of the tests, due to the low volatility and high viscosity of the test material. No mortality was noted, and all animals fully recovered following depuration. The lack of mortality at concentrations at or above the limit dose of 2.0 mg/L indicates a relatively low order of toxicity for these substances.

Data Assessment and Test Plan for Acute Mammalian Toxicity

Adequate acute toxicity studies have been conducted with four structural analogs of decene tetramer/trimer. These studies involved two species of laboratory animals (rats or rabbits) and three routes of exposure (oral, dermal, and inhalation). The data consistently demonstrate a low order of acute toxicity for PAOs derived from C10 and C12 alpha olefins. The similarity in the low order of toxicity for these substances is consistent with their similar chemical structure and physicochemical properties and supports the scientific justification for read across to decene tetramer/trimer. Consequently, no additional acute toxicity testing is proposed for the HPV Challenge Program.

Table 1. Summary of Existing Acute Mammalian Toxicity Data for Decene Tetramer/Trimer and Structural Analogs

PRODUCT	Oral LD50 (rats)	Dermal LD50 (rats/rabbits)	Inhalation LC50 (rats)
1-Decene, tetramer, mixed with 1-decene trimer, hydrogenated (CAS 68649-12-7)	RA	RA	RA
1-Decene homopolymer, hydrogenated (CAS 68037-01-4)*	--	--	>2.5 mg/L (4 hr)
1-Decene/1-dodecene copolymer, hydrogenated (CAS 151006-60-9)*	>5 g/kg+	>2 g/kg+ (rats)	>5.0 mg/L (4 hr)
1-Octene, 1-decene, 1-dodecene copolymer, hydrogenated (CAS 163149-28-8)*	>2 g/kg	>2 g/kg+ (rabbits)	--
1-Dodecene trimer, hydrogenated (CAS 151006-62-1)*	>5 g/kg	>2 g/kg (rats)	>5.06 mg/L (4hr)

* Not an HPV material; included to support assessment.
+ Based on ExxonMobil Chemical Company Material Safety Data Sheet information – robust summary is not provided.

3. Genotoxicity of Decene Tetramer/Trimer

Summary of Genotoxicity Data

A summary of the genotoxicity information for analogous PAOs (decene homopolymer, octene/decene/dodecene copolymer, dodecene trimer; and decene/dodecene copolymer [*prepared from 10% C12 and 90% C10 alpha olefins; approx. 33% trimer and 51% tetramer, 16% pentamer and higher*]) is presented in Table 2. Either bacterial or mammalian gene mutation assays, *in vitro* chromosomal aberration assays, or *in vivo* chromosomal aberration assays have been conducted for these substances. Neither mutagenicity nor clastogenicity were exhibited by any of these substances in the referenced *in vivo* or *in vitro* tests, with or without metabolic activation.

Bacterial Gene Mutation Assay

Analogous PAOs (decene homopolymer, octene/ decene/dodecene copolymer, dodecene trimer, and decene/dodecene copolymer) have all been adequately tested in Bacterial Reverse Mutation Tests. Decene homopolymer (with 10 ppm of an antioxidant) was also negative in the modified bacterial gene mutation assay. All tested substances were

negative for mutagenic activity, with and without metabolic activation.

Mammalian Cell Gene Mutation Assay

A structural analog of decene tetramer/trimer, dodecene trimer, was negative in the Chinese hamster ovary cell HGPRT gene mutation assay, with and without metabolic activation.

In vitro Chromosomal Aberration Assay

Three structurally analogous PAOs (decene homopolymer, octene/decene/dodecene copolymer, and dodecene trimer) were adequately tested in *in vitro* chromosomal aberration assays. Decene homopolymer and octene/decene/dodecene copolymer were tested in the Chinese hamster ovary (CHO) cell assay. Dodecene trimer was evaluated in the *in vitro* chromosome aberration test in human lymphocytes. The results of these studies, performed with and without metabolic activation of the test material, were negative for clastogenicity.

In vivo Chromosomal Aberration Assays

The structural analog, decene homopolymer, has been adequately tested in an *in vivo* chromosomal aberration assay. Male and female rats treated dermally with test material at doses of 800 and 2000 mg/kg/day, five days per week for 13 weeks were used to assess cytotoxicity to red blood cells. The bone marrow and peripheral blood were collected from the rats following the 13-week period. The test material was not cytotoxic to red blood cell formation, nor did it induce a statistically significant increase in the formation of micronucleated PCEs or NCEs in bone marrow or peripheral blood cells of dermally treated rats. Decene/dodecene copolymer and dodecene trimer were also negative in mouse micronucleus assays after intraperitoneal (i.p.) administration.

Data Assessment and Test Plan for Genotoxicity

Four structural analogs of decene tetramer/trimer have been tested for genotoxicity (viz., gene mutations and chromosomal aberrations). The assays included gene mutations in bacterial cells, *in vitro* chromosomal aberrations in mammalian cells, and *in vivo* chromosomal aberrations in rats and mice. The data consistently demonstrated no evidence of genotoxicity regardless of metabolic activation. This suggests that decene tetramer/trimer and all structural analogs lack genotoxicity due to their similarity in chemical structures and physicochemical properties and supports scientific justification for bridging data gaps within this HPV Challenge Program.

By bridging these data, decene tetramer/trimer has been evaluated adequately for genotoxicity, and no additional testing is proposed for the HPV Challenge Program**.**

Table 2. Summary of Existing Genotoxicity Data for Decene Tetramer/Trimer and

Structural Analogs

PRODUCT	Bacterial Gene Mutation Test	Mammalian Cell Gene Mutation Test	In Vitro Mammalian Cell Chromosome Aberration Tests	In Vivo Mammalian Chromosome Aberration Test
1-Decene, tetramer, mixed with 1-decene trimer, hydrogenated (CAS 68649-12-7)	RA	RA	RA	RA
1-Decene homopolymer, hydrogenated (CAS 68037-01-4)*	Negative+	--	Negative+ (CHO cell assay)	Negative (Rat micronucleus, repeat dermal)
1-Decene/1-dodecene copolymer, hydrogenated (CAS 151006-60-9)*	Negative	--	--	Negative (Mouse micronucleus, i.p.)
1-Octene, 1-decene, 1-dodecene copolymer, hydrogenated (CAS 163149-28-8)*	Negative	--	Negative (CHO cell assay)	--
1-Dodecene trimer, hydrogenated* (CAS 151006-62-1)	Negative	Negative (CHO HGPRT)	Negative (Human lymphocyte assay)	Negative (Mouse micronucleus, i.p.)

* Not an HPV material, included to support assessment.
RA Read across.
\+ Based on ExxonMobil Chemical Company Material Safety Data Sheet Information – robust summaries are not provided.

4. Repeated-Dose Toxicity of Decene Tetramer/Trimer

Summary of Repeated-Dose Toxicity Data

The HPV Challenge Program requires that a repeated-dose toxicity study and a reproductive toxicity study be performed or bridged to structurally analogous substances. No adequate repeated-dose toxicity studies have been located for decene tetramer/trimer; however, adequate data for repeated-dose toxicity are available for three structural analogs of this product.

One 28-day oral toxicity study in rats, one 90-day dermal and two 90-day dietary studies in rats, and a dermal carcinogenicity study in mice exist for the analogous substance, decene homopolymer. A rat oral combined reproductive toxicity and 91-day systemic toxicity study was also conducted with decene homopolymer [see Reproductive/Developmental section for reproductive toxicity phase information]. In addition, 28-day rat oral toxicity studies exist for two structurally analogous substances (dodecene trimer and octene/decene/dodecene copolymer); and a 90-day rat dermal toxicity study exists for octene/decene/dodecene copolymer.

Results from these studies show a low order of repeated dose toxicity and are presented in

Table 3.

Repeated-Dose Dermal Toxicity

Octene/decene/dodecene copolymer was applied to clipped backs of male and female rats five days per week for approximately four weeks at dose levels of 0 (untreated control), 125, 500, and 2000 mg/kg/day. In addition, two satellite groups, one exposed to octene/decene/dodecene copolymer at 2000 mg/kg/day and one that received no treatment, were observed for two weeks following the four weeks of dosing. The test material produced no signs of skin irritation at the site of exposure. After four weeks of dosing, there was a slight decrease in body weight gain for males dosed at 2000 mg/kg/day. Female weight gain was not affected. No microscopic changes were associated with treatment. The NOEL for systemic toxicity for this study was 500 mg/kg/day. However, the observed changes in body weight and hematology were marginal and were only observed in the satellite group and not the treatment group. Therefore, the NOAEL for systemic toxicity in this study was 2000 mg/kg/day.

Decene homopolymer was applied to the skin of Sprague-Dawley rats, five days a week for thirteen weeks at dose levels of 800 and 2000 mg/kg/day. Body weights of the high-dose males were slightly less than those of the controls (9% less). There were no other indications of systemic toxicity. The substance caused only slight effects (slight flaking) at the application site on the skin. Based on the above results, the NOAEL for decene homopolymer following topical application in rats is 2000 mg/kg/day.

Decene homopolymer produced no treatment-related tumors in C3H mice treated with a 50 μl/application twice weekly for 104 weeks. In addition, survival (56%) was greater than in any other group, including the untreated control.

Repeated-Dose Oral Toxicity

Decene homopolymer was evaluated in a 28-day oral gavage rangefinding toxicity study at dose levels of 0, 500, 2500, and 5000 mg/kg/day in Sprague-Dawley rats. No significant clinical signs indicative of systemic toxicity were observed. No gross pathological changes were noted. Histological evaluation of the liver revealed no adverse effects. Based on the above results, the NOAEL for 1-decene homopolymer is 5,000 mg/kg/day in Sprague-Dawley rats.

Decene homopolymer was evaluated in a 90-day oral (feeding) toxicity study at dose levels of 500, 5000 and 20,000 ppm in Sprague-Dawley rats. No clinical signs indicative of systemic toxicity were observed. None of the major organ systems showed any detectable treatment-related changes. Based on the above results, the NOAEL for 1-decene homopolymer is 20,000 ppm in Sprague-Dawley rats.

Decene homopolymer was evaluated in a 90-day oral (feeding) toxicity study at dose levels of 200 and 20,000 ppm in Fischer 344 rats. No clinical signs indicative of systemic toxicity were observed. No adverse effects were observed for the hematology results with the substance. Marginal serum chemistry effects were observed for the male rats following 90 days of treatment with the substance in the diet at 20,000 ppm. None of the major organ systems showed any detectable treatment-related changes. Based on the above results, the NOAEL for decene homopolymer is 20,000 ppm in Fischer 344 rats.

A rat oral combined reproductive toxicity and systemic toxicity study was also conducted with decene homopolymer, with Sprague-Dawley rats at levels of 0, 100, 500, and 1000 mg/kg/day [see Reproductive/Developmental section for reproductive toxicity phase information]. In this study, parental animals were dosed for 4 weeks prior to mating and during mating (males and females), during gestation and to day 20 post-partum (females). The offspring were dosed for 91 days starting on day 22 post-partum. No treatment related toxicity was observed in the F0 male and female rats. The F1 pups did not demonstrate any test article related toxicity during parturition and lactation. In the F1 rats during the 91-day toxicity phase, repeated oral exposure of decene homopolymer produced no evidence of any adverse effects on clinical observations, organ weights, gross or histopathology, clinical chemistry or hematology endpoints. Based on these data, the NOAEL for repeated dose toxicity was 1000 mg/kg/day, the highest concentration tested.

Oral administration of the structural analog, decene trimer, to Sprague-Dawley rats for a period of twenty-eight consecutive days at a dose level of 1000 mg/kg/day produced no treatment-related changes in the parameters measured. The NOAEL was 1000 mg/kg/day.

Data Assessment and Test Plan for Repeated-Dose Toxicity

Eight repeated-dose toxicity studies using two different animal species, rats and mice, and oral and dermal routes of administration have been conducted with three structural analogs of decene tetramer/trimer. These data suggest that decene tetramer/trimer and all structural analogs exhibit a low order of toxicity following repeated applications, due to their similarity in chemical structures and physicochemical properties, and support scientific justification for bridging data gaps within this HPV Challenge Program.

By bridging these data, decene tetramer/trimer has been evaluated adequately for repeated exposure toxicity, and no additional testing is proposed for the HPV Challenge Program**.**

Table 3. Summary of Existing Repeated-Dose Toxicity Data for Decene Tetramer/Trimer and Structural Analogs

PRODUCT	28-Day (Sprague-Dawley rat)	90-Day (Sprague-Dawley/Fischer 344 rat)	Chronic (mouse)
1-Decene, tetramer, mixed with 1-decene trimer, hydrogenated (CAS 68649-12-7)	RA	RA	RA

PRODUCT	28-Day (Sprague-Dawley rat)	90-Day (Sprague-Dawley/Fischer 344 rat)	Chronic (mouse)
1-Decene homopolymer, hydrogenated (CA 68037-01-4)*	NOAEL >5000 mg/kg/day (Rangefinding Study, Sprague-Dawley rat) (oral gavage)	NOAEL >20,000 ppm (Sprague-Dawley rats) (Dietary) NOAEL >2000 mg/kg/day+ (Sprague-Dawley rats) (Dermal) NOAEL >20,000 ppm (Fischer 344 rats) (Dietary) NOAEL >1000 mg/kg/day (Sprague-Dawley rats) (oral gavage)	104-Week Dermal Carcinogenicity (Negative)
1-Octene, 1-decene, 1-dodecene copolymer, hydrogenated (CAS 163149-28-8)*		NOAEL 2000 mg/kg/day (Sprague-Dawley) (Dermal)	--
1-Dodecene trimer, hydrogenated* (CAS 151006-62-1)	NOAEL >1000 mg/kg/day (oral gavage)	--	--

* Not an HPV material, included to support assessment.
RA Read across.
\+ Based on ExxonMobil Chemical Company Material Safety Data Sheet Information – robust summary is not provided.

5. Reproductive/Developmental Toxicity of Decene Tetramer/Trimer

No adequate reproductive or developmental toxicity studies have been located for decene tetramer/trimer; however, data are available for the structural analog, decene homopolymer. Results from these studies show a low order of reproductive/ developmental toxicity and are presented in Table 4.

Developmental Toxicity

Decene homopolymer (with 10 ppm of an antioxidant) was administered once daily on gestation days 0-19 via dermal application to presumed-pregnant rats at doses of 0, 800, and 2000 mg/kg/day. Dermal administration of the test material did not adversely affect parameters of reproductive performance during gestation, nor did it adversely affect *in utero* survival and development of the offspring. The NOAEL in this study for developmental

parameters was 2000 mg/kg/day.

Reproductive Toxicity

A rat oral combined reproductive toxicity and systemic toxicity study was conducted with decene homopolymer. This study with rats was conducted as part of a 91-day toxicity study with offspring of parents administered decene homopolymer by oral gavage. Parents and offspring received decene homopolymer at 0, 100, 500, and 1000 mg/kg/day. The parental males were dosed for a minimum of 4 weeks prior to mating and throughout the 15-day breeding period. Parental females were dosed for 4 weeks prior to mating, through pregnancy and until sacrifice at day 20 post-partum. The offspring were dosed for a minimum of 91 days starting on day 22 post-partum. No effects on fertility were seen. The NOAEL for reproductive toxicity was 1000 mg/kg/day, the highest concentration tested. The lack of effects on fertility in this study or effects on reproductive organs in this or other subchronic studies with closely related chemicals indicates that decene tetramer/trimer is unlikely to exert effects on reproduction.

Table 4. Summary of Existing Reproductive/Developmental Toxicity Data for Decene Tetramer/Trimer and Structural Analogs

PRODUCT	Reproductive (Rat)	Developmental (Rat)
1-Decene, tetramer, mixed with 1-decene trimer, hydrogenated (CAS 68649-12-7)	RA	RA
1-Decene homopolymer (CAS 68037-01-4)*	Combined Repeated Exposure and Reproduction Oral Toxicity Study NOAEL 1000 mg/kg/day (Oral gavage)	Maternal/Fetal NOAEL = 2000 mg/kg/day (Dermal)

* Not an HPV material, included to support assessment.
RA Read across.

Data Assessment and Test Plan for Reproductive/Developmental Toxicity

No studies have been located where decene tetramer/trimer was tested for reproductive/developmental toxicity. However, a dermal developmental toxicity study and an oral reproductive toxicity study with rats were conducted with a structural analog, 1-decene homopolymer. In addition, toxicity to reproductive organs has been assessed in repeated-dose studies with structural analogs. These data are considered adequate to address the potential developmental/reproductive toxicity of decene tetramer/trimer and no additional developmental/reproductive toxicity tests are proposed.

IV. EVALUATION OF EXISTING PHYSICOCHEMICAL AND ENVIRONMENTAL FATE DATA AND PROPOSALS FOR ADDRESSING THESE ENDPOINTS

A. Physicochemical Properties

Physicochemical data (i.e., melting point, boiling point, vapor pressure, water solubility, and Kow) for decene tetramer/trimer will be calculated using the EPIWIN© model (EPIWIN, 1999), as discussed in the EPA document titled *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* (U.S. EPA, 1999a). In addition, measured data for some of these endpoints will also be provided for decene tetramer/trimer or structural analogs. Where possible, the measured and calculated data will be presented together in robust summaries for comparative purposes. Table 5 lists selected measured physicochemical data as the data appeared on the material safety data sheets for decene tetramer/trimer or analogous chemicals.

Table 5. Selected Physical Properties of Decene Tetramer/Trimer and Analogs

CAS NUMBER	CHEMICAL NAME	BOILING POINT (° C)	VAPOR PRESSURE (mm Hg @ 20° C)	SPECIFIC GRAVITY	WATER SOLUBILITY	LOG K_{ow}
68649-12-7	1-Decene tetramer/trimer	>316	<0.1	0.82	< 1 ppt* 2.3 E^{-10} ppm**	>7.0*

* Read across value for an analogous chemical, 1-dodecene trimer, hydrogenated

** Estimated value for a C30 oligomer (Log K_{ow} = 14.6). Estimated using WSKOW v.1.36 of EPIWIN v.3.04.

B. Biodegradation

Biodegradation data were developed for decene tetramer/trimer using the EPA Shake Flask Method (EPA 560/6-82-003, CG-2000) with an unacclimated sewage/soil inoculum. At initial test material concentrations of 10 and 20 mg of carbon per liter, 54% and 49% biodegradation, respectively, were measured after 28 days (Mobil Oil Corporation, 1992c). Although these data do not meet the criteria to be considered readily biodegradable, the data show that decene tetramer/trimer can biodegrade to a great extent, which suggests that it will not persist in the environment.

C. Photodegradation, Hydrolysis, and Fugacity

1. Photodegradation – Photolysis (Direct)

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may undergo a transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First-order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (1977). The UV light absorption of decene tetramer/trimer will be evaluated to identify if it has the potential to degrade in solution. A technical discussion will be prepared for this endpoint that summarizes the results of this evaluation.

2. Photodegradation – Photolysis (Indirect)

Photodegradation can be measured (U.S. EPA, 1999b) (EPA identifies OECD test guideline 113 as a test method) or estimated using models accepted by the EPA (U.S. EPA, 1999a). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect degradation. AOPs can be calculated using a computer model.

Polyalphaolefins, such as the one in this test plan, have a low potential to volatilize to air. In air, volatilized chemicals can undergo reactions with photosensitized oxygen in the form of ozone and hydroxyl radicals. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. Although decene tetramer/trimer is not expected to partition to the air to a significant degree based on its low vapor pressure, this calculation will be performed for a representative chemical structure of this product, and the results summarized within the technical discussion on direct photolysis.

3. Stability in Water (Hydrolysis)

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985). Stability in water can be measured (US EPA, 1999b) (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (US EPA, 1999a).

The product in this test plan is a hydrocarbon. That is, it consists entirely of carbon and hydrogen. As such, it is not expected to hydrolyze at a measurable rate. A technical document will be prepared that discusses the potential hydrolysis rate of this product, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

4. Chemical Distribution in the Environment (Fugacity Modeling)

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The U.S. EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (Mackay, 1996). EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* (US EPA, 1999b), which was prepared as guidance for the HPV Program.

In its document, EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments (air, soil, water, suspended sediment, sediment, biota) within a unit world.

Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. This model will be used to calculate distribution values for a representative structure of the product in this test plan. A computer model, EPIWIN, version 3.04 (EPIWIN, 1999), will be used to calculate the properties needed to run the Level I EQC model that are not available as measured values.

V. EVALUATION OF AQUATIC TOXICITY DATA

Aquatic toxicity endpoints for the HPV Program include acute toxicity to a freshwater fish and invertebrate, and toxicity to a freshwater alga. Decene tetramer/trimer is not expected to produce acute toxic effects to freshwater fish and invertebrates, or toxic effects to algae, based on data developed for this product and an analogous product, octene/decene/dodecene copolymer (Table 6).

Table 6. Summary of Aquatic Toxicity Data for PAO Anchor Studies

PRODUCT	Freshwater Fish Acute (96-hr)	Marine Fish Acute (96-hr)	Marine Invertebrate Acute (96-hr)	Freshwater Invertebrate Acute (48-hr)	Freshwater Alga (72-hr)
1-Decene, tetramer, mixed with 1-dodecene trimer, hydrogenated	LL_0 = 5010 mg/L (RA)	LL_0 = 5002 mg/L	LL_0 = >5002 mg/L	EL_0 = 5220 mg/L(RA)	EL_0 = 5220 mg/L (RA)

RA Read across data from 1-octene, 1-decene, 1-dodecene copolymer, hydrogenated.

Experimental toxicity test results for decene tetramer/trimer are reported for a marine fish, sheepshead minnow (*Cyprinodon variegatus*), and a marine invertebrate, mysid shrimp (*Mysidopsis bahia*) (Mobil Oil Corporation, 1992a,b). Additional experimental toxicity test results for octene/decene/dodecene copolymer are also reported for a freshwater fish, rainbow trout (*Oncorhynchus mykiss*), a freshwater invertebrate (*Daphnia magna*), and a freshwater alga (*Selenastrum capricornutum*, now known as *Pseudokirchneriella subcapitata*) (Stonybrook, 1994a,b,c). The data from these studies show that these products do not produce toxicity to these organisms for the selected endpoints. The reason for the lack of toxicity is most likely due to the low water solubility of these products.

The water solubility of decene tetramer/trimer is very low. Although no data specifically for this product has been located, there are data from a soil adsorption/desorption study for a product similar to decene tetramer/trimer. The results from this study show that octene/decene/dodecene copolymer has a water solubility less than 0.4 mg/L (Stonybrook, 1995), which was the lowest limit of detectability in this study. The water solubility of another similar product, dodecene trimer, was determined to be <1 ppt, the limit of detection in the assay (Seary, 2000). By structural comparison, these data suggest that decene tetramer/trimer also has low water solubility. This is not unexpected for a product whose chemical components range in molecular weight from approximately 422 for a C30

component to 562 for a C40 component.

VI. TEST PLAN SUMMARY

Sufficient data exist for decene tetramer/trimer and analogous chemicals to adequately characterize the HPV Program human health effects, aquatic toxicity, and biodegradation endpoints for decene tetramer/trimer. No additional testing is proposed for these endpoints.

The following modeling and technical discussions will be developed for the physicochemical properties and other environmental fate endpoints:

- Calculate physicochemical data as described in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* for selected chemical components of the product in this test plan. Provide measured data where readily available.
- Prepare a technical discussion on the potential of the polyalphaolefin product in this test plan to photodegrade. Calculate AOP values for a representative chemical structure of the product in this test plan.
- Prepare a technical discussion on the potential of the polyalphaolefin product in this test plan to hydrolyze.
- Calculate fugacity data for a representative chemical structure of the product in this test plan.

The assessment plan for 1-decene, tetramer, mixed with 1-decene trimer, hydrogenated, is presented in Table 7.

Robust summaries of existing studies (except as noted in Tables 1-3) of health effects, aquatic toxicity, biodegradation, and physicochemical data are attached (Appendix 1). Summaries of the other environmental fate and physicochemical endpoints will be developed once the data and analyses have been completed. This test plan is expected to provide adequate data to characterize the human health effects, physicochemical, and environmental fate and effects endpoints for decene tetramer/trimer under the HPV Program.

Table 7. Assessment Plan for 1-Decene, Tetramer, Mixed with 1-Decene Trimer, Hydrogenated, Under the HPV Program (Except as noted in Tables 1-3, robust summaries for existing studies are provided in Appendix 1).

Chemical	Human Health Effects						Ecotoxicity			Physico-chem-ical	Environmental Fate			
	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Develop-mental	Repro-duction	Acute Fish	Acute Inver-tebrate	Alga Toxicity		Photo-degra-dation	Hydro-lysis	Fugacity	Biodeg-radation
1-Decene, Tetramer, Mixed with 1-Decene Trimer, Hydrogenated [85% trimer, 13% tetramer, 2% pentamer and higher] CAS # 68649-12-7	**RA**	**RA**	**RA**	**RA**	**RA**	**RA**	√	√	**RA**	**CM/M**	**CM/TD**	**TD**	**CM**	√
1-Decene, Homopolymer, Hydrogenated CAS # 68037-01-4	√	--	√	√	√	√	--	--	--	--	--	--	--	--
1-Decene/1-Dodecene Copolymer, Hydrogenated [C10 oligomers: approximately 33% trimer (C30), 51% tetramer (C40), 16% pentamer (C50) and higher; and C 12 oligomers] CAS # 151006-60-9	√	√	√	--	--	--	--	--	--	--	--	--	--	--
1-Octene, 1-Decene, 1-Dodecene Copolymer, Hydrogenated CAS # 163149-28-8	√	√	√	√	--	--	√	√	√	√*	--	--	--	--
1-Dodecene Trimer, Hydrogenated CAS # 151006-62-1	√	√	√	√	--	--	√	√	√	√**	--	--	--	--

√ Adequate existing data available
√* Water solubility
√** Water solubility and $Log_{10}P_{ow}$
TD Technical discussion proposed
CM Computer modeling proposed
M Identify measured data where available (a robust summary for water solubility is provided with this test plan)
Shaded areas denote non-HPV substances
RA Read across data from structural analogs: 1-octene, 1-decene, 1-dodecene copolymer, hydrogenated; 1-dodecene trimer, hydrogenated; 1-decene/1-dodecene copolymer and/or 1-decene homopolymer, hydrogenated (see Tables 1- 6)

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